Discrete Applied Mathematics 160 (2012) 1152–1163

Contents lists available at SciVerse ScienceDirect

Discrete Applied Mathematics

journal homepage: www.elsevier.com/locate/dam

On the reciprocal degree distance of graphs[☆]

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ARTICLE INFO

Article history:
Received 28 June 2011
Received in revised form 28 November 2011
Accepted 30 November 2011
Available online 23 December 2011

Keywords:
Distance (in graphs)
Degree distance
Reciprocal degree distance
Bounds
Extremal graphs

ABSTRACT

In this paper, we study a new graph invariant named reciprocal degree distance (RDD), defined for a connected graph G as vertex-degree-weighted sum of the reciprocal distances, that is, $RDD(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v)) \frac{1}{d_G(u,v)}$. The reciprocal degree distance is a weight version of the Harary index, just as the degree distance is a weight version of the Wiener index. Our main purpose is to investigate extremal properties of reciprocal degree distance. We first characterize among all nontrivial connected graphs of given order the graphs with the maximum and minimum reciprocal degree distance, respectively. Then we characterize the nontrivial connected graph with given order, size and the maximum reciprocal degree distance as well as the tree, unicyclic graph and cactus with the maximum reciprocal degree distance, respectively. Finally, we establish various lower and upper bounds for the reciprocal degree distance in terms of other graph invariants including the degree distance, Harary index, the first Zagreb index, the first Zagreb coindex, pendent vertices, independence number, chromatic number and vertex-, and edge-connectivity.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For a graph G, we let $d_G(v)$ be the degree of a vertex v in G and $d_G(u, v)$ be the distance between two vertices u and v in G.

One of the oldest and well-studied distance-based graph invariants associated with a connected graph G is the Wiener number $W(G)$, also termed as *Wiener index* in chemical or mathematical chemistry literature, which is defined [25] as the sum of distances over all unordered vertex pairs in G, namely,

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v).$$

This equation was introduced by Haruo Hosoya [13], although the concept has been introduced by late Harry Wiener. However, the approach by Wiener is applicable only to acyclic structures, whilst Hosoya matrix definition allowed the Wiener index to be used for any structure.

Another distance-based graph invariant, defined [17,19] in a fully analogous manner to Wiener index, is the *Harary index*, which is equal to the sum of reciprocal distances over all unordered vertex pairs in G, that is,

$$H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d_G(u, v)}.$$

☆ Supported by NNSF of China (no. 11171273), SRF of HIT (No. HGA1010), and sponsored by Qing Lan Project of Jiangsu Province, PR China.
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doi:10.1016/j.dam.2011.11.032

Dobrynin and Kochetova [8] and Gutman [10] independently proposed a vertex-degree-weighted version of Wiener index called *degree distance* or *Schultz molecular topological index*, which is defined for a connected graph G as

$$DD(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v))d_G(u, v).$$

The interested readers may consult [7,11,12,15] for Wiener index, [6,18,19,28,27,29,32] for Harary index and [4,5,9,16,20,22,24,23,21] for degree distance.

Noting that the degree distance is a degree-weight version of the Wiener index and bearing in mind that the relation between Wiener index and Harary index, we introduce here a new graph invariant named reciprocal degree distance, which can be seen as a degree-weight version of Harary index, that is,

$$\mathrm{RDD}(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v))\frac{1}{d_G(u, v)}. \tag{1}$$

In this paper, we mainly study extremal properties of reciprocal degree distance. We organize this paper as follows. In Section 2, we characterize among all nontrivial connected graphs of given order the graphs with the maximum and minimum reciprocal degree distance, respectively. In Section 3, we characterize the nontrivial connected graph with given order, size and the maximum reciprocal degree distance as well as the tree, unicyclic graph and cactus with the maximum reciprocal degree distance, respectively. Moreover, we establish various lower and upper bounds for the reciprocal degree distance in terms of other graph invariants including the degree distance, Harary index, the first Zagreb index, the first Zagreb coindex, pendent vertices, independence number, chromatic number and vertex-, and edge-connectivity.

Before proceeding, we introduce some further notation and terminology. A vertex in a graph is said to be a *pendent vertex* if it is of degree one. The *diameter* of a connected graph is the greatest distance between any pair of vertices in this graph. The *eccentricity* of a vertex v in a graph G is defined to be $ec_G(v) = \max\{d_G(u, v)|u \in V(G)\}$. Denoted by P_n, S_n and K_n the path, star and complete graphs on n vertices, respectively. Let tK_1 be the union of t copies of K_1. A connected graph is said to be a *tree*, if it has no cycles, and is said to be a *unicyclic graph* if it has exactly a cycle. Other notation and terminology not defined here will conform to those in [3].

2. Connected graphs with the maximum and minimum RDD

We first give two useful lemmas used later.

Lemma 1. *Let G be a connected graph with at least three vertices.*

(i) *If G is not isomorphic to K_n, then $\mathrm{RDD}(G) < \mathrm{RDD}(G + e)$, where $e \in E(\overline{G})$;*
(ii) *If G has an edge e not being a cut edge, then $\mathrm{RDD}(G) > \mathrm{RDD}(G - e)$.*

Proof. We first prove (i) holds. Suppose that G is not a complete graph. Then there exists a pair of vertices u and v in G such that $uv \in E(\overline{G})$. It is obvious that $d_G(x, y) \geq d_{G+uv}(x, y)$ for any pair of vertices x and y in G. Also, we have $d_G(u, v) > 1 = d_{G+uv}(u, v)$. Moreover, $d_{G+uv}(w) \geq d_G(w)$ for any w in G. By Eq. (1), we have $\mathrm{RDD}(G) < \mathrm{RDD}(G + uv)$, as claimed.

Now, we consider (ii). Since the edge e is not a cut edge in G, we have $G - e$ is connected and not isomorphic to the complete graph of the same order. Thus, by (i), we have $\mathrm{RDD}(G - e) < \mathrm{RDD}((G - e) + e) = \mathrm{RDD}(G)$, as desired. □

Let $\widehat{D}_G(u) = \sum_{v\in V(G)\setminus\{u\}} \frac{1}{d_G(u,v)}$. Then we can rewrite Eq. (1) as

$$\mathrm{RDD}(G) = \sum_{u\in V(G)} d_G(u)\widehat{D}_G(u). \tag{2}$$

The above Eq. (2) is frequently used throughout the paper.

Lemma 2. *Suppose that H is a nontrivial connected graph and u is a vertex in H. Let G_1 (resp., G_2) be a graph obtained by identifying the vertex u of H with a non-pendent vertex (resp., a pendent vertex) of the path P_l ($l \geq 3$). Then $\mathrm{RDD}(G_1) > \mathrm{RDD}(G_2)$.*

Proof. For each vertex x in $V(H)\setminus\{u\}$, we clearly have $d_{G_1}(x) = d_H(x) = d_{G_2}(x)$. Also, $d_{G_1}(u) = d_H(u)+2$, $d_{G_2}(u) = d_H(u)+1$.

We label all vertices of path P_l ($l \geq 3$) as $v_1, \ldots, v_l$ and assume in G_1 that $u = v_i$ for some $2 \leq i \leq l - 1$. Then we have $u = v_1$(or v_l) in G_2.

For $1 \leq j \leq l$, we let $d_{ij} = d_{P_l}(v_i, v_j)$. Rearranging these d_{ij}'s and relabeling them as d'_{ij}'s such that $d'_{i1} \leq d'_{i2} \leq \cdots \leq d'_{il}$. Then, $d'_{ij} \leq j - 1$ for $j = 1, \ldots, l$. In particular, $d'_{i1} = 0$.

For each vertex x in $V(H)\setminus\{u\}$, we have

$$\begin{aligned}\widehat{D}_{G_1}(x) &= \sum_{y\in V(H)\setminus\{u,x\}}\frac{1}{d_H(x,y)}+\sum_{y\in V(P_l)}\frac{1}{d_G(x,y)}\\ &= \sum_{y\in V(H)\setminus\{u,x\}}\frac{1}{d_H(x,y)}+\sum_{1\le j\le l}\frac{1}{d_H(x,u)+d_{P_l}(v_j,v_i)}\\ &= \sum_{y\in V(H)\setminus\{u,x\}}\frac{1}{d_H(x,y)}+\frac{1}{d_H(x,u)}+\sum_{1\le j\le l, j\ne i}\frac{1}{d_H(x,u)+d_{P_l}(v_j,v_i)}\\ &= \sum_{y\in V(H)\setminus\{u,x\}}\frac{1}{d_H(x,y)}+\frac{1}{d_H(x,u)}+\sum_{2\le j\le l}\frac{1}{d_H(x,u)+d'_{ij}}\\ &\ge \sum_{y\in V(H)\setminus\{u,x\}}\frac{1}{d_H(x,y)}+\frac{1}{d_H(x,u)}+\sum_{2\le j\le l}\frac{1}{d_H(x,u)+j-1}\\ &= \widehat{D}_{G_2}(x).\end{aligned}$$

Thus,

$$\sum_{x\in V(H)\setminus\{u\}} d_{G_1}(x)\widehat{D}_{G_1}(x) \ge \sum_{x\in V(H)\setminus\{u\}} d_{G_2}(x)\widehat{D}_{G_2}(x). \tag{3}$$

In the following, we shall prove that $\sum_{j=1}^{l} d_{G_1}(v_j)\widehat{D}_{G_1}(v_j) \ge \sum_{j=1}^{l} d_{G_2}(v_j)\widehat{D}_{G_2}(v_j)$.

For each $1\le j\le l$, we have

$$\widehat{D}_{G_1}(v_j) = \widehat{D}_{P_l}(v_j) + \sum_{x\in V(H)\setminus\{u\}}\frac{1}{d_{P_l}(v_j,v_i)+d_H(u,x)} \tag{4}$$

and

$$\widehat{D}_{G_2}(v_j) = \widehat{D}_{P_l}(v_j) + \sum_{x\in V(H)\setminus\{u\}}\frac{1}{d_{P_l}(v_j,v_1)+d_H(u,x)}. \tag{5}$$

For each $1\le j\le l$, we let δ'_{ij} denote the degree of vertex corresponding to d'_{ij}. Then we have, $\delta'_{i1}=d_H(u)+2$ and $\delta'_{il}=1$. It is obvious that there exists a positive integer j_0 in the interval $[2, l-1]$ such that $\delta'_{ij_0}=1$.

For $1\le j\le l$, we let $d_{1j}=d_{P_l}(v_j,v_1)$. Then, $d_{11}<d_{12}<\cdots<d_{1l}$. Obviously, $d_{G_2}(v_1)=d_H(u)+1$ and $d_{G_2}(v_l)=1$. For the above chosen j_0, we have $d_{G_2}(v_{j_0})=2$.

For $2\le j\le l-1$ and $j\ne j_0$, we have $\delta'_{ij}=d_{G_2}(v_j)=2$.

From the definition above it follows that $d'_{ij}\le d_{1j}$ for each $j=1,\ldots,l$.

For each given x in $V(H)\setminus\{u\}$, we let $f_x(j)=d'_{ij}+d_H(u,x)$ and $g_x(j)=d_{1j}+d_H(u,x)$. Then we have

$$f_x(j)\le g_x(j) \tag{6}$$

for each x and $j=1,\ldots,l$.

Note that for each $2\le j\le l$ and $j\ne i$, $d_{G_1}(v_j)=d_{G_2}(v_j)=d_{P_l}(v_j)$. By means of Eqs. (4) and (5),

$$\begin{aligned}\sum_{j=1}^{l} d_{G_1}(v_j)\widehat{D}_{G_1}(v_j) &= \sum_{j=1}^{l} d_{G_1}(v_j)\widehat{D}_{P_l}(v_j)+\sum_{j=1}^{l}\delta'_{ij}\sum_{x\in V(H)\setminus\{u\}}\frac{1}{f_x(j)}\\ &= (d_H(u)+2)\widehat{D}_{P_l}(v_i)+1\cdot\widehat{D}_{P_l}(v_1)+\sum_{j=2,j\ne i}^{l} d_{P_l}(v_j)\widehat{D}_{P_l}(v_j)\\ &\quad+\sum_{j=2,j\ne j_0}^{l}\delta'_{ij}\sum_{x\in V(H)\setminus\{u\}}\frac{1}{f_x(j)}+\delta'_{ij_0}\sum_{x\in V(H)\setminus\{u\}}\frac{1}{f_x(j_0)}+\delta'_{i1}\sum_{x\in V(H)\setminus\{u\}}\frac{1}{d_H(u,x)}\end{aligned}$$

and

$$\sum_{j=1}^{l} d_{G_2}(v_j)\widehat{D}_{G_2}(v_j) = \sum_{j=1}^{l} d_{G_2}(v_j)\widehat{D}_{P_l}(v_j)+\sum_{j=1}^{l} d_{G_2}(v_j)\sum_{x\in V(H)\setminus\{u\}}\frac{1}{g_x(j)}$$

$$= (d_H(u)+1)\widehat{D}_{P_l}(v_1) + 2\widehat{D}_{P_l}(v_i) + \sum_{j=2, j\neq i}^{l} d_{P_l}(v_j)\widehat{D}_{P_l}(v_j)$$
$$+ \sum_{j=2, j\neq j_0}^{l} d_{G_2}(v_j) \sum_{x\in V(H)\setminus\{u\}} \frac{1}{g_x(j)} + d_{G_2}(v_{j_0}) \sum_{x\in V(H)\setminus\{u\}} \frac{1}{g_x(j_0)} + d_{G_2}(v_1) \sum_{x\in V(H)\setminus\{u\}} \frac{1}{d_H(u,x)}.$$

By above analysis and Eq. (6), we have

$$\sum_{j=2, j\neq j_0}^{l} \delta'_{ij} \sum_{x\in V(H)\setminus\{u\}} \frac{1}{f_x(j)} \geq \sum_{j=2, j\neq j_0}^{l} d_{G_2}(v_j) \sum_{x\in V(H)\setminus\{u\}} \frac{1}{g_x(j)}. \tag{7}$$

By means of Eqs. (6) and (7), we obtain

$$\sum_{j=1}^{l} d_{G_1}(v_j)\widehat{D}_{G_1}(v_j) - \sum_{j=1}^{l} d_{G_2}(v_j)\widehat{D}_{G_2}(v_j)$$
$$\geq d_H(u)(\widehat{D}_{P_l}(v_i) - \widehat{D}_{P_l}(v_1)) + \delta'_{ij_0} \sum_{x\in V(H)\setminus\{u\}} \frac{1}{f_x(j_0)} - d_{G_2}(v_{j_0}) \sum_{x\in V(H)\setminus\{u\}} \frac{1}{g_x(j_0)}$$
$$+ (d_H(u)+2) \sum_{x\in V(H)\setminus\{u\}} \frac{1}{d_H(u,x)} - (d_H(u)+1) \sum_{x\in V(H)\setminus\{u\}} \frac{1}{d_H(u,x)}$$
$$= d_H(u)(\widehat{D}_{P_l}(v_i) - \widehat{D}_{P_l}(v_1)) + \sum_{x\in V(H)\setminus\{u\}} \frac{1}{f_x(j_0)} - 2\sum_{x\in V(H)\setminus\{u\}} \frac{1}{g_x(j_0)} + \sum_{x\in V(H)\setminus\{u\}} \frac{1}{d_H(u,x)}$$
$$\geq d_H(u)(\widehat{D}_{P_l}(v_i) - \widehat{D}_{P_l}(v_1)) - \sum_{x\in V(H)\setminus\{u\}} \frac{1}{g_x(j_0)} + \sum_{x\in V(H)\setminus\{u\}} \frac{1}{d_H(u,x)}$$
$$\geq d_H(u)(\widehat{D}_{P_l}(v_i) - \widehat{D}_{P_l}(v_1)).$$

In the following, we will prove that $\widehat{D}_{P_l}(v_i) > \widehat{D}_{P_l}(v_1)$ for each given $2 \leq i \leq l-1$.

Obviously, $\widehat{D}_{P_l}(v_1) = \sum_{k=1}^{l-1} \frac{1}{k}$. Let d'_{ij} be defined as before. Since $0 = d'_{i1} \leq d'_{i2} \leq \cdots \leq d'_{il}$ and $d'_{ij} \leq j-1$, we have $\widehat{D}_{P_l}(v_i) = \sum_{j=2}^{l} \frac{1}{d'_{ij}} \geq \sum_{j=2}^{l} \frac{1}{j-1} = \widehat{D}_{P_l}(v_1)$ for each $2 \leq i \leq l-1$. Also, we clearly have $\frac{1}{d'_{i3}} = 1 > \frac{1}{2}$. So, $\widehat{D}_{P_l}(v_i) > \widehat{D}_{P_l}(v_1)$ for each $2 \leq i \leq l-1$.

By discussion above, we have arrived at

$$\sum_{j=1}^{l} d_{G_1}(v_j)\widehat{D}_{G_1}(v_j) > \sum_{j=1}^{l} d_{G_2}(v_j)\widehat{D}_{G_2}(v_j). \tag{8}$$

From the combination of Eqs. (3) and (8) it follows readily that $\mathrm{RDD}(G_1) > \mathrm{RDD}(G_2)$ as claimed. □

For graphs G_1 and G_2 as introduced in Lemma 2, we call the graph operation $G_1 \Longrightarrow G_2$ the *α-transformation* on G_1.

By means of Lemmas 1 and 2, we are able to characterize connected graphs with the maximum and minimum RDD, respectively. More precisely, we have the following result.

Theorem 1. *Among all nontrivial connected graphs of order n, the graphs with the maximum and minimum RDD are K_n and P_n, respectively.*

Proof. The case of $n = 2$ is trivial. So we suppose that $n \geq 3$.

We first prove that K_n is maximal with respect to RDD. If G is not a complete graph, then we can repeatedly add edges into G until we obtain $G \cong K_n$. By Lemma 1, $\mathrm{RDD}(G) \leq \mathrm{RDD}(K_n)$, with equality if and only if $G \cong K_n$.

Now, let us prove that P_n is minimal with respect to RDD. Suppose first that G is not isomorphic to a tree. Let $T(G)$ be a spanning tree of G. It then follows from Lemma 1 that $\mathrm{RDD}(G) > \mathrm{RDD}(T(G))$. So we need only to consider the case of G is a tree. If $G \ncong P_n$, then we can repeatedly employ α-transformation on G and we must obtain the path P_n in the end. By Lemma 2, each step of α-transformation will result in a new tree with a strictly smaller RDD than that of the previous one. Then $\mathrm{RDD}(G) > \mathrm{RDD}(P_n)$, as desired. □

3. Relation with other graph parameters

In this section, we shall establish various bounds for RDD in terms of other graph parameters.

From the definition of RDD, we can obtain the following several direct results.

Theorem 2. *Let G be a nontrivial connected graph. Then*

$$\mathrm{RDD}(G) \le DD(G)$$

with equality if and only if $G \cong K_n$.

Proof. For any two vertices u and v in G, we clearly have $\frac{1}{d_G(u,v)} \le d_G(u, v)$ with equality if and only if $d_G(u, v) = 1$. So,

$$\begin{aligned}\mathrm{RDD}(G) &\le \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v))d_G(u, v)\\ &= DD(G).\end{aligned}$$

Thus, $\mathrm{RDD}(G) \le DD(G)$ with equality if and only if for any two vertices u and v in G, $d_G(u, v) = 1$, that is, $G \cong K_n$. □

Recall that $M_1(G) = \sum_{u\in V(G)}(d_G(u))^2$ is the *first Zagreb index* (see [14,26,30,31]) and $\overline{M}_1(G) = \sum_{uv\notin E(G)}(d_G(u) + d_G(v))$ is the *first Zagreb coindex* (see [1,2]). By means of these notations, we state the following result.

Theorem 3. *Let G be a nontrivial connected graph. Then*

$$\mathrm{RDD}(G) \le M_1(G) + \overline{M}_1(G)$$

with equality if and only if $G \cong K_n$.

Proof. For any two vertices u and v in G, we clearly have $\frac{1}{d_G(u,v)} \le 1$ with equality if and only if $d_G(u, v) = 1$. So,

$$\begin{aligned}\mathrm{RDD}(G) &\le \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v))\\ &= \sum_{uv\in E(G)} (d_G(u) + d_G(v)) + \sum_{uv\notin E(G)} (d_G(u) + d_G(v))\\ &= \sum_{x\in V(G)} (d_G(x))^2 + \overline{M}_1(G)\\ &= M_1(G) + \overline{M}_1(G).\end{aligned}$$

Thus $\mathrm{RDD}(G) \le M_1(G) + \overline{M}_1(G)$ with equality if and only if for any two vertices u and v in G, $d_G(u, v) = 1$, that is, $G \cong K_n$. □

Let $\Delta(G)$ and $\underline{\Delta}(G)$ denote the maximum and minimum vertex-degree in a graph G.

Theorem 4. *Let G be a nontrivial connected graph. Then*

$$2\underline{\Delta}(G)H(G) \le \mathrm{RDD}(G) \le 2\Delta(G)H(G)$$

with either equality if and only if G is a regular graph.

Proof. For each vertex x in G, we have $\underline{\Delta}(G) \le d_G(x) \le \Delta(G)$. So,

$$2\underline{\Delta}(G) \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d_G(u, v)} \le \mathrm{RDD}(G) \le 2\Delta(G) \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d_G(u, v)},$$

that is,

$$2\underline{\Delta}(G)H(G) \le \mathrm{RDD}(G) \le 2\Delta(G)H(G).$$

This completes the proof. □

Theorem 5. *Let G be a nontrivial connected graph. Then*

$$\mathrm{RDD}(G) \ge \frac{(M_1(G) + \overline{M}_1(G))^2}{DD(G)}$$

with equality if and only if $G \cong K_n$.

Proof. By the definition of degree distance and reciprocal degree distance, we get

$$\begin{aligned} DD(G)\cdot \mathrm{RDD}(G) &= \left(\sum_{\{u,v\}\subseteq V(G)} (d_G(u)+d_G(v))d_G(u,v)\right)\cdot\left(\sum_{\{u,v\}\subseteq V(G)} (d_G(u)+d_G(v))\frac{1}{d_G(u,v)}\right) \\ &\geq \left(\sum_{\{u,v\}\subseteq V(G)} (d_G(u)+d_G(v))\right)^2 \\ &= \left(\sum_{uv\in E(G)} (d_G(u)+d_G(v)) + \sum_{uv\notin E(G)} (d_G(u)+d_G(v))\right)^2 \\ &= (M_1(G)+\overline{M}_1(G))^2. \end{aligned}$$

So, $\mathrm{RDD}(G) \geq \frac{(M_1(G)+\overline{M}_1(G))^2}{DD(G)}$ with equality if and only if $d_G(u,v)$ is a constant, that is, $G \cong K_n$. This completes the proof. □

Now, we characterize connected graphs with n vertices, m edges and extremal RDD.

Theorem 6. *Let G be a connected graph of order $n \geq 2$ and size $m \geq 1$. Then*

$$\frac{2(n-1)m}{d} + \frac{(d-1)M_1(G)}{d} \leq \mathrm{RDD}(G) \leq (n-1)m + \frac{M_1(G)}{2}$$

with either equality if and only if $d \leq 2$, where d is the diameter of G.

Proof. First, let us prove that the right-hand side inequality holds. For each vertex x in G, we have

$$\begin{aligned} \widehat{D}_G(x) &= d_G(x) + \sum_{y\in V(G)\setminus N_G[x]} \frac{1}{d_G(x,y)} \\ &\leq d_G(x) + \frac{n-d_G(x)-1}{2} \\ &= \frac{n+d_G(x)-1}{2}, \end{aligned}$$

where the equality is attained if and only if $ec_G(x) \leq 2$.

From Eq. (2) and above inequality it follows immediately that

$$\begin{aligned} \mathrm{RDD}(G) &= \sum_{x\in V(G)} d_G(x)\widehat{D}_G(x) \\ &\leq \sum_{x\in V(G)} d_G(x)\left(\frac{n+d_G(x)-1}{2}\right) \\ &= \frac{n-1}{2}\sum_{x\in V(G)} d_G(x) + \frac{1}{2}\sum_{x\in V(G)} (d_G(x))^2 \\ &= (n-1)m + \frac{M_1(G)}{2}, \end{aligned}$$

where the equality is attained if and only if for each x, $ec_G(x) \leq 2$.

So, $\mathrm{RDD}(G) \leq (n-1)m + \frac{M_1(G)}{2}$ with equality if and only if the diameter of G is at most 2, as desired.

Now, we turn to the left-hand side inequality.

For each vertex x in G,

$$\begin{aligned} \widehat{D}_G(x) &= d_G(x) + \sum_{y\in V(G)\setminus N_G[x]} \frac{1}{d_G(x,y)} \\ &\geq d_G(x) + \frac{n-d_G(x)-1}{d} \\ &= \frac{n+(d-1)d_G(x)-1}{d}, \end{aligned}$$

where the equality is attained if and only if for any $y \in V(G)\setminus N_G[x]$, $d_G(x,y) = d$, implying that $d \leq 2$.

Therefore,

$$\begin{aligned}\mathrm{RDD}(G) &\geq \sum_{x\in V(G)} d_G(x)\left\lceil \frac{n+(d-1)d_G(x)-1}{d}\right\rceil \\ &= \frac{n-1}{d}\sum_{x\in V(G)} d_G(x) + \frac{d-1}{d}\sum_{x\in V(G)} (d_G(x))^2 \\ &= \frac{2(n-1)m}{d} + \frac{(d-1)M_1(G)}{d},\end{aligned}$$

where the equality is attained if and only if $d \leq 2$.

This completes the proof. □

A *cactus* is a connected graph each of whose blocks is either a cycle or an edge. If a cactus has no cycles, then it is just a tree, and if it has exactly a cycle, then it is a unicyclic graph.

For $0 \leq k \leq \frac{n-1}{2}$, we let G_n^k be an n-vertex k-cycle cactus obtained from the n-vertex star by adding k independent edges among $n-1$ pendent vertices.

In the following, we shall give a sharp upper bound for RDD of k-cycle cactus. Before proceeding any further, let us cite a result of [33] as the following lemma.

Lemma 3. *Let G be an n-vertex k-cycle cactus with $0 \leq k \leq \frac{n-1}{2}$. Then*

$$M_1(G) \leq n^2 - n + 6k$$

with equality if and only if $G \cong G_n^k$.

Theorem 7. *Let G be an n-vertex k-cycle cactus with $0 \leq k \leq \frac{n-1}{2}$. Then*

$$\mathrm{RDD}(G) \leq \frac{3n^2 + (2k-5)n + 4k + 2}{2}$$

with equality if and only if $G \cong G_n^k$.

Proof. Note that G has $n+k-1$ edges. By Theorem 6 and Lemma 3, we have

$$\begin{aligned}\mathrm{RDD}(G) &\leq (n-1)(n+k-1) + \frac{M_1(G)}{2} \\ &\leq (n-1)(n+k-1) + \frac{M_1(G_n^k)}{2} \\ &= (n-1)(n+k-1) + \frac{n^2-n+6k}{2} \\ &= \frac{3n^2 + (2k-5)n + 4k + 2}{2}.\end{aligned}$$

The above first equality holds if and only if the diameter of G is 2 and the second one holds if and only if $G \cong G_n^k$.

Note that G_n^k has diameter 2. Thus, $\mathrm{RDD}(G) \leq \frac{3n^2+(2k-5)n+4k+2}{2}$ with equality if and only if $G \cong G_n^k$, completing the proof. □

By Theorem 7, we immediately have the following results for RDD of trees and unicyclic graphs, respectively.

Corollary 1. *Let T be a tree on $n \geq 2$ vertices. Then*

$$\mathrm{RDD}(T) \leq \frac{3n^2 - 5n + 2}{2},$$

with equality if and only if $T \cong S_n$.

Corollary 2. *Let G be a unicyclic graph on $n \geq 3$ vertices. Then*

$$\mathrm{RDD}(G) \leq \frac{3n^2 - 3n + 6}{2},$$

with equality if and only if $G \cong G_n^1$.

Let K_n^p denote the graph obtained by attaching p pendent edges to a vertex of K_{n-p}. We first prove the following result.

Lemma 4. *Let G be an n-vertex connected graph with p pendent vertices. Then*

$$M_1(G) \le n^3 - (3p-1)n^2 + (3p^2+6p+1)n - p^3 - 3p^2 - 2p - 1$$

with equality if and only if $G \cong K_n^p$.

Proof. Suppose that $G_{\max}$ is a graph chosen among all connected graphs with n vertices and p pendent vertices such that it has the maximum first Zagreb index. Let $D(G_{\max}) = \{x_1, x_2, \ldots, x_n\}$ denote the degree sequence of $G_{\max}$. If we label all pendent vertices of $G_{\max}$ as $v_1, \ldots, v_p$, then $G[V(G_{\max}) \setminus \{v_1, \ldots, v_p\}]$, the subgraph of $G_{\max}$ induced by vertices in $V(G_{\max}) \setminus \{v_1, \ldots, v_p\}$ must be a clique in $G_{\max}$, for otherwise, we can obtain a new graph with a strictly larger first Zagreb index than that of $G_{\max}$ by adding edges into $G_{\max}$.

Note that the degree sequence $D(K_n^p) = \{n-1, \underbrace{n-p-1, \ldots, n-p-1}_{n-p-1}, \underbrace{1, \ldots, 1}_{p}\}$. If $G_{\max} \ncong K_n^p$, then there must exist a pair (x_i, x_j), in $G_{\max}$ with $n-p \le x_i \le x_j \le n-2$. We construct a new n-vertex and p-pendent vertex connected graph G' by replacing the pair (x_i, x_j) in $G_{\max}$ by the pair $(x_i - 1, x_j + 1)$. It is easy to obtain that $M_1(G') > M_1(G_{\max})$, a contradiction to our choice of $G_{\max}$.

Then $G_{\max} \cong K_n^p$. Also, $M_1(K_n^p) = (n-1)^2 + p + (n-p-1)^3 = n^3 - (3p-1)n^2 + (3p^2+6p+1)n - p^3 - 3p^2 - 2p - 1$. So we are done. □

Theorem 8. *Let G be an n-vertex connected graph with p pendent vertices. Then*

$$\mathrm{RDD}(G) \le \frac{3n^3 - 8pn^2 + (7p^2+17p+3)n - 2p^3 - 7p^2 - 7p - 2}{4}$$

with equality if and only if $G \cong K_n^p$.

Proof. Let G^* be a connected graph with n vertices and p pendent vertices $v_1, \ldots, v_p$ satisfying that $G[V(G^*) \setminus \{v_1, \ldots, v_p\}]$, the subgraph of G^* induced by vertices in $V(G^*) \setminus \{v_1, \ldots, v_p\}$, is a clique in G^*. We need only to consider the upper bound for RDD of G^* by Lemma 1.

It is obvious that G^* has $p + \binom{n-p}{2} = p + \frac{(n-p)(n-p-1)}{2}$ edges. By Theorem 6 and Lemma 4, we have

$$\begin{aligned}
\mathrm{RDD}(G^*) &\le (n-1)m + \frac{M_1(G^*)}{2} \\
&= \frac{(n-1)\left[\frac{(n-p)^2+3p-n}{2}\right]}{2} + \frac{M_1(G^*)}{2} \\
&\le (n-1)\left[\frac{(n-p)^2+3p-n}{2}\right] + \frac{M_1(K_n^p)}{2} \\
&= \frac{3n^3 - 8pn^2 + (7p^2+17p+3)n - 2p^3 - 7p^2 - 7p - 2}{4}.
\end{aligned}$$

The first equality holds if and only if the diameter of G^* is at most 2 and the second one holds if and only if $G^* \cong K_n^p$.

Note that K_n^p has diameter 2. So, $\mathrm{RDD}(G) \le \frac{3n^3-8pn^2+(7p^2+17p+3)n-2p^3-7p^2-7p-2}{4}$ with equality if and only if $G \cong K_n^p$. This completes the proof. □

A vertex subset S of a graph G is said to be an *independent set* of G, if the subgraph induced by S is an empty graph. Then $\beta = \max\{|S| : S \text{ is an independent set of } G\}$ is said to be the *independence number* of G.

Theorem 9. *Let G be an n-vertex connected graph with independence number β. Then*

$$\mathrm{RDD}(G) \le n^3 - (\beta+1)n^2 - \left(\frac{3}{2}\beta^2 - \frac{3}{2}\beta - 1\right)n + \frac{1}{2}\beta^3 + \frac{1}{2}\beta^2 - \beta$$

with equality if and only if $G \cong \beta K_1 \vee K_{n-\beta}$.

Proof. Let $G_{\max}$ be a graph chosen among all n-vertex connected graphs with independence number β such that $G_{\max}$ has the largest RDD. Let S be a maximal independent set in $G_{\max}$ with $|S| = \beta$. Since adding edges into a graph will increase its RDD by Lemma 1, each vertex x in S is adjacent to every vertex y in $G_{\max} - S$. Moreover, the subgraph induced by vertices in $G_{\max} - S$ is a clique in $G_{\max}$. So $G_{\max} \cong \beta K_1 \vee K_{n-\beta}$. An elementary calculation gives $\mathrm{RDD}(\beta K_1 \vee K_{n-\beta}) = (n-\beta)(n-1)^2 + \beta(n-\beta)[(n-\beta) + (\beta-1)\frac{1}{2}] = n^3 - (\beta+1)n^2 - (\frac{3}{2}\beta^2 - \frac{3}{2}\beta - 1)n + \frac{1}{2}\beta^3 + \frac{1}{2}\beta^2 - \beta$, as claimed. □

Denote by $T_{n,t}$ the *Turán graph*, a complete t-partite graph of order n with $|n_i - n_j| \le 1$, where $n_i, i = 1, \ldots, t$, is the number of vertices in the ith partite set of $T_{n,t}$.

Theorem 10. *Let G be an n-vertex connected graph with chromatic number χ such that $n = q\chi + p$, $0 \le p \le \chi - 1$. Then*

$$\mathrm{RDD}(G) \le n^3 - (3q+2)n^2 + \left(\frac{3}{2}q^2\chi + \frac{3}{2}q\chi + \frac{3}{2}q^2 + \frac{5}{2}q + 1\right) n - q(q+1)^2\chi$$

with equality if and only if $G \cong T_{n,\chi}$.

Proof. Let $G_{\max}$ be a graph chosen among all n-vertex connected graphs with chromatic number χ such that $G_{\max}$ has the largest RDD. Because the addition of edges into a graph increases its RDD, we must have $G_{\max} \cong \overline{K_{n_1}} \vee \overline{K_{n_2}} \vee \cdots \vee \overline{K_{n_\chi}}$, where n_i is the number of vertices in the ith partite set.

By the definition of RDD, we obtain

$$\begin{aligned}\mathrm{RDD}(G_{\max}) &= \sum_{i=1}^{\chi} n_i(n-n_i)\left[(n-n_i) + (n_i-1)\cdot\frac{1}{2}\right]\\ &= \sum_{i=1}^{\chi} n_i(n-n_i)\left(n - \frac{n_i}{2} - \frac{1}{2}\right)\\ &= \frac{1}{2}\sum_{i=1}^{\chi} n_i^3 + \frac{1}{2}(1-3n)\sum_{i=1}^{\chi} n_i^2 + \frac{2n^3-n^2}{2}.\end{aligned}$$

Suppose that $G_{\max} \ncong T_{n,\chi}$. Then there exists $n_j \ge n_i + 2$ for some $1 \le i, j \le \chi$. We let $G' = \overline{K_{n_1}} \vee \cdots \vee \overline{K_{n_i+1}} \vee \cdots \vee \overline{K_{n_j-1}} \vee \cdots \vee \overline{K_{n_\chi}}$.

Then

$$\begin{aligned}\mathrm{RDD}(G') - \mathrm{RDD}(G_{\max}) &= \frac{1}{2}[(n_j-1)^3 + (n_i+1)^3 - n_j^3 - n_i^3] + \frac{1-3n}{2}[(n_j-1)^2 + (n_i+1)^2 - n_j^2 - n_i^2]\\ &= \frac{1}{2}(-3n_j^2 + 3n_i^2 + 3n_j + 3n_i) + \frac{1-3n}{2}(2n_i + 2 - 2n_j)\\ &= \frac{n_i+1-n_j}{2}(3n_j + 3n_i + 2 - 6n).\end{aligned}$$

Since $G_{\max}$ is connected, we have $\chi \ge 2$, and then $n_i < n_j \le n-1$. Thus, $3n_j + 3n_i + 2 - 6n < 0$. Note that $n_i + 1 - n_j < 0$; thus we have $\mathrm{RDD}(G') > \mathrm{RDD}(G_{\max})$, a contradiction to our choice of $G_{\max}$. So we have $G_{\max} \cong T_{n,\chi}$. Moreover, we have

$$\begin{aligned}\mathrm{RDD}(T_{n,\chi}) &= p(q+1)(n-q-1)\left[(n-q-1) + q\cdot\frac{1}{2}\right] + (\chi-p)q(n-q)\left[(n-q) + (q-1)\cdot\frac{1}{2}\right]\\ &= \sum_{i=1}^{\chi} n_i(n-n_i)\left(n - \frac{n_i}{2} - \frac{1}{2}\right)\\ &= n^3 - (3q+2)n^2 + \left(\frac{3}{2}q^2\chi + \frac{3}{2}q\chi + \frac{3}{2}q^2 + \frac{5}{2}q + 1\right)n - q(q+1)^2\chi.\end{aligned}$$

This completes the proof. □

The *vertex-connectivity* is the minimum number of vertices whose deletion from a connected graph disconnects it, and the *edge-connectivity* is the minimum number of edges whose deletion from a connected graph disconnects it.

Let G and H be two vertex-disjoint graphs. The *join* of graphs G and H, denoted by $G \vee H$, is defined as a graph whose vertex set is $V(G) \cup V(H)$ and edge set is $E(G) \cup E(H) \cup \{xy | x \in V(G), y \in V(H)\}$.

Theorem 11. *Let G be an n-vertex connected graph with vertex-connectivity k. Then*

$$\mathrm{RDD}(G) \le n^3 - \frac{9}{2}n^2 + \left(2k + \frac{13}{2}\right)n + \frac{1}{2}k^2 - \frac{5}{2}k - 3$$

with equality if and only if $G \cong K_k \vee (K_1 + K_{n-k-1})$.

Proof. We choose $G_{\max}$ to be a graph such that $G_{\max}$ has the largest RDD within all connected graphs with n vertices and vertex-connectivity k. Let C be a vertex-cut in $G_{\max}$ such that $|C| = k$ and let $G_{\max} - C = G_1 \cup G_2 \cup \ldots G_t$ $(t \ge 2)$. By Lemma 1, we must have $t = 2$, for otherwise, we can adding edges between any two components, resulting in a new graph G' with vertex-connectivity k and a strictly larger RDD than that of $G_{\max}$, a contradiction to our choice of $G_{\max}$.

The same reason leads us to that both G_1 and G_2 are cliques of $G_{\max}$, that the subgraph of $G_{\max}$ induced by C is a clique, and that any vertex in $G_1 \cup G_2$ is adjacent to each vertex in C. Let n_i denote the order of G_i. Thus, we have $G_{\max} \cong K_k \vee (K_{n_1} + K_{n_2})$.

Assume without loss of generality that $n_2 \geq n_1$. If $n_1 = 1$, then the result follows readily. Suppose now that $n_2 \geq n_1 \geq 2$. By Eq. (2), we obtain

$$\begin{aligned}
\mathrm{RDD}(G_{\max}) &= \sum_{x\in V(G_1)} d_{G_{\max}}(x)\widehat{D}_{G_{\max}}(x) + \sum_{x\in V(G_2)} d_{G_{\max}}(x)\widehat{D}_{G_{\max}}(x) + \sum_{x\in V(C)} d_{G_{\max}}(x)\widehat{D}_{G_{\max}}(x)\\
&= n_1(n-n_2-1)\left[(n-n_2-1)+\frac{1}{2}n_2\right] + k(n-1)^2 + n_2(n-n_1-1)\left[(n-n_1-1)+\frac{1}{2}n_1\right]\\
&= \left(n^3-2n^2+n\right) + \left(3-\frac{5}{2}n-\frac{1}{2}k\right)n_1n_2.
\end{aligned}$$

Let $G' = K_k \vee (K_{n_1-1} + K_{n_2+1})$. Then

$$\begin{aligned}
\mathrm{RDD}(G') - \mathrm{RDD}(G_{\max}) &= \left(3-\frac{5}{2}n-\frac{1}{2}k\right)[(n_1-1)(n_2+1)-n_1n_2]\\
&= \left(3-\frac{5}{2}n-\frac{1}{2}k\right)(n_1-n_2-1) > 0,
\end{aligned}$$

a contradiction to our choice of $G_{\max}$.

Thus, $G_{\max} \cong K_k \vee (K_1 + K_{n-k-1})$. An elementary calculation gives $\mathrm{RDD}(K_k \vee (K_1 + K_{n-k-1})) = n^3 - \frac{9}{2}n^2 + (2k + \frac{13}{2})n + \frac{1}{2}k^2 - \frac{5}{2}k - 3$, completing the proof. □

In the following theorem, we show that $K_k \vee (K_1 \cup K_{n-1-k})$ also maximizes RDD among all n-vertex connected graphs with edge-connectivity k.

Theorem 12. *Let G be an n-vertex connected graph with edge-connectivity k. Then*

$$\mathrm{RDD}(G) \leq n^3 - \frac{9}{2}n^2 + \left(2k + \frac{13}{2}\right)n + \frac{1}{2}k^2 - \frac{5}{2}k - 3$$

with equality if and only if $G \cong K_k \vee (K_1 + K_{n-k-1})$.

Proof. Suppose that $G_{\max}$ is a graph chosen among all n-vertex connected graphs with edge-connectivity k such that $G_{\max}$ has the maximum RDD. We intend to prove that $G_{\max} \cong K_k \vee (K_1 \cup K_{n-1-k})$ below.

Let $\{e_1, \ldots, e_k\}$ be a k-edge cut in $G_{\max}$, and let $G_{\max} - \{e_1, \ldots, e_k\} = G_1 \cup G_2$. Since adding edges into a graph increases its RDD by Lemma 1, both G_1 and G_2 must be complete graphs. Denote by n_i the order of G_i $(i = 1, 2)$.

We claim that $n_i = 1$ or $n_i \geq k$ $(k \geq 2)$. Suppose that $n_i \geq 2$. On one hand, G_i has $\frac{n_i(n_i-1)}{2}$ edges, as G_i is a complete graph. On the other hand, the sum of degrees of all vertices in G_i is at least n_ik (because the minimum degree of $G_{\max}$ is at least k), and thus, G_i has at least $\frac{n_ik-k}{2}$ edges. So,

$$\frac{n_i(n_i-1)}{2} \geq \frac{n_ik-k}{2},$$

that is,

$$n_i^2 - (k+1)n_i + k \geq 0,$$

implying that $n_i \geq k$, as claimed.

Suppose without loss of generality that $n_2 \geq n_1$. If $n_1 = 1$, then $G_{\max}$ is just the graph $K_k \vee (K_1 \cup K_{n-1-k})$, as claimed.

Assume now that $n_2 \geq n_1 \geq k$.

Firstly, we assume that there is a vertex, say v, in $V(G_{\max})$, of degree k. Let $v_1, \ldots, v_k$ be neighbors of v. Write $A = \{v_1, \ldots, v_k\}$ and $B = V(G_{\max}) \setminus \{v, v_1, \ldots, v_k\}$.

If $G[A\cup B]$, the subgraph of $G_{\max}$ induced by $A\cup B$, is the complete graph K_{n-1}, then $G_{\max} \cong K_k \vee (K_1 \cup K_{n-1-k})$, as claimed.

Suppose that $G[A \cup B] \ncong K_{n-1}$. Then we can add an edge, say uv, between a vertex u in A and a vertex v in B and the resulting graph is denoted by G'. Clearly, the edge-connectivity of G' is k. But then, we have $\mathrm{RDD}(G_{\max}) < \mathrm{RDD}(G')$ by Lemma 1, a contradiction to the choice of $G_{\max}$.

So we may suppose that $d_{G_{\max}}(v) \geq k+1$ for any vertex v in $G_{\max}$. Then we must have $n_2 \geq n_1 \geq k+1$. In fact, if $n_1 = k$, then each vertex in G_1 is adjacent to at least two vertices in G_2, since each vertex in $G_{\max}$ is of degree $\geq k+1$. But then the number of edges between G_1 and G_2 is at least $2k$, a contradiction.

From [14], we know that if G is an n-vertex connected graph with edge-connectivity k, then

$$M_1(G) \leq n^3 - 5n^2 + (2k+8)n + k^2 - 3k - 4$$

with equality if and only if $G \cong K_k \vee (K_1 + K_{n-k-1})$.

Note that $G_{\max}$ has $\binom{n_1}{2}+\binom{n_2}{2}+k$ edges. Then by Theorem 6,

$$\begin{aligned}
\mathrm{RDD}(G_{\max}) &\le (n-1)\left[\binom{n_1}{2}+\binom{n_2}{2}+k\right]+\frac{M_1(G_{\max})}{2}\\
&\le (n-1)\left[\binom{n_1}{2}+\binom{n_2}{2}+k\right]+\frac{n^3-5n^2+(2k+8)n+k^2-3k-4}{2}\\
&= n^3-\frac{7}{2}n^2+\left(2k+\frac{9}{2}\right)n+\frac{1}{2}k^2-\frac{5}{2}k-2-(n-1)n_1n_2.
\end{aligned}$$

Since $n_2 \ge n_1 > k$ and $n_1+n_2=n$, we have $n_1n_2 > k(n-k)$.
Thus,

$$\begin{aligned}
\mathrm{RDD}(G_{\max}) &< n^3-\frac{7}{2}n^2+\left(2k+\frac{9}{2}\right)n+\frac{1}{2}k^2-\frac{5}{2}k-2-(n-1)k(n-k)\\
&= n^3-\left(k+\frac{7}{2}\right)n^2+\left(k^2+3k+\frac{9}{2}\right)n-\frac{1}{2}k^2-\frac{5}{2}k-2.
\end{aligned}$$

But then,

$$\begin{aligned}
&\mathrm{RDD}(K_k\vee(K_1+K_{n-k-1}))-\mathrm{RDD}(G_{\max})\\
&> \left[n^3-\frac{9}{2}n^2+\left(2k+\frac{13}{2}\right)n+\frac{1}{2}k^2-\frac{5}{2}k-3\right]-\left[n^3-\left(k+\frac{7}{2}\right)n^2+\left(k^2+3k+\frac{9}{2}\right)n-\frac{1}{2}k^2-\frac{5}{2}k-2\right]\\
&= (k-1)n^2-(k^2+k-2)n+k^2-1\\
&\ge (k-1)n\cdot[2(k+1)]-(k^2+k-2)n+k^2-1(\text{because } n=n_1+n_2\ge 2k+2)\\
&= k^2n-kn+k^2-1>0,
\end{aligned}$$

a contradiction to our choice of $G_{\max}$ once again.

From discussion above, we have completed the proof. $\square$

Let $f(k)=n^3-\frac{9}{2}n^2+(2k+\frac{13}{2})n+\frac{1}{2}k^2-\frac{5}{2}k-3$. It is easy to see that $f(k)$ is a strictly increasing function. It then follows immediately from Theorems 11 and 12 the following consequence.

Corollary 3. *Let G be a connected graph on n vertices with vertex-connectivity (or edge-connectivity) at most k. Then*

$$\mathrm{RDD}(G)\le n^3-\frac{9}{2}n^2+\left(2k+\frac{13}{2}\right)n+\frac{1}{2}k^2-\frac{5}{2}k-3$$

with equality if and only if $G\cong K_k\vee(K_1+K_{n-k-1})$.

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